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Formation of simple bio-molecules during collapse of an interstellar cloud – a preliminary analysis

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Abstract : More than 120 molecules have been observed in molecular clouds, more than half of which are organic. Some of them, especially those which contain C and N are important because they could be the pre-cursors of more complex bio-molecules We explore the possibilities of formation of these molecules during interstellar cloud collapse and star formation During collapse, the density and temperature of the gas increase, thereby increasing the reaction rates of the constituent atoms and molecules. Presence of grains and metallic catalysts may increase the reaction rate further. We therefore discuss in details the effects of grains in forming H_2 molecules in the cloud We show how the mass fraction of simple molecules such as HCN, H_2O, NH_3 *etc.* varies with radial distance of a collapsing cloud.

Keywords : Molecular clouds, star formation, bio-molecules.

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1. Introduction

Our earth is not a special place in this Universe. However, it is a planet with favorable conditions where complex bio-molecules could form and life could evolve. Chemical analysis of various carbonaceous chondrites like Murchison meteorite shows that plenty of organic molecules including eight types of biologically significant amino acids are present in them. In Didwana-Rajod meteorite, which is believed to be 4.5 billion years old and was analysed by an Indian team [1] also found three amino acids. This team concluded that these are originated from the outer space. Furthermore, the spectral analysis of interstellar lines shows 124 types of molecules. Among them, nearly 80 species are organic and are present in the dense interstellar medium. All these motivate us to study the formation of bio-molecules in space. Our procedure is to couple hydrodynamic equations with chemical evolution of the interstellar medium following Chakrabarti and Chakrabarti [2] and check if at least simple bio-molecules are produced in the process. To achieve this goal, a major concern has been to include the grain chemistry in a fully consistent way so as to produce H_2 molecules from H on the grain surface. Gould and Salpeter [3] pointed out that observed H_2 molecules could not possibly come from gas phase alone and dust grains may have to be used as catalysts. Subsequently, Hollenbach, Werner and Salpeter [4] computed the sticking probability and mobility of H on the grain surface and produced H_2 through recombination of hydrogen. Temperature-programmed desorption method to determine the recombination co-efficients was used by Pirronello *et al* [5] and was analyzed by Katz *et al* [6]. We employ these co-efficients in our work for the production of molecular hydrogen which is used in our computation of bio-molecule formation.

As the gas collapses, the density increases and more and more H_2 is produced on the grain surface. At the same time, the temperature of the gas and the grain rises due to trapping of the gravitational potential energy. This is

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rigorously true, especially in the adiabatic phase when the rotational velocity becomes so significant that centrifugal barrier slows down the radial collapse.

In the present paper, we concentrate on the introduction of the grain chemistry and formation of simple molecules, such as H_2, HCN, N_2O *etc.* In our next article, we shall use this knowledge to compute more complex biomolecules directly related to life. In the Section 2, we present a brief introduction to hydrodynamic condition in a collapsing cloud. In Section 3, we describe our procedure for $H + H \rightarrow H_2$ reaction on the grain surface. In Section 4, we discuss the chemical evolution of the interstellar cloud. In Section 5, we present the result of our numerical analysis to show how the composition of the flow changes during collapse. Finally, in Section 6, we present our concluding remarks.

2. Brief introduction to hydrodynamic study

A generic interstellar cloud may have two distinct regions. One is diffused having density ρ ~1–1000/cm^3 and temperature 80 K and the other is the dense molecular cloud having ρ ~10^3–10^6/cm^3 and temperature around 10 K. Typical size of a molecular cloud is ~10–10^4 pc and the average lifetime is ~10– 20 Myr. Initially, the cloud passes through an isothermal phase $T = T_0$ = constant when the heat generated collapse is radiated away through the optically thin region. In this phase, $\rho \sim r^{-2}$ [7] and the velocity is constant. In presence of rotation, centrifugal barrier is formed at $r = r_c$, where centrifugal force balances gravity. At this stage the collapse is disk-like and the opacity becomes high enough to trap radiations, the cloud collapses adiabatically with r. Density falls off as r in this region [8]. Following Shu *et al* [9], we compute the density, temperature and velocity distribution inside the cloud and following Chakrabarti and Chakrabarti [2], we carry out the chemical evolution at the same time. Results will be presented below.

3. Formation of H_2 by grain chemistry

Grains are very important constituents of interstellar medium. The effect of these grains is that they influence the production of hydrogenated species such as H_2O, NH_3, CH_4 *etc.* due to high mobility of atomic hydrogen on their cold surfaces. Therefore, we need to take into account the rates of such grain surface reactions in the reaction network as given below :

$H + H \rightarrow H_2$, $H_2 + H_2 \rightarrow H_3^+ + H$, $H + OH \rightarrow H_2O$, $C^+ + H_2 \rightarrow CH_2^+ + h\nu$, $CH_2^+ + H_2 \rightarrow CH_3^+ + H$, $CH_3^+ + H_2 \rightarrow CH_5 + h\nu$, $CH_5 + e^- \rightarrow CH_4 + H$. Tunneling reactions with H_2 could occur once $H_2 >> H$. Direct production of bigger and heavier species does not get influenced very much by grains.

To simplify our computation, we do not assume that the grains have all possible sizes. Mathis *et al* [10] proposed a power-law distribution for the grains. More accurate description of the distribution was presented by Weingartner and Draine [11]. Following this, we find that essentially there are three types of grain sizes : one with

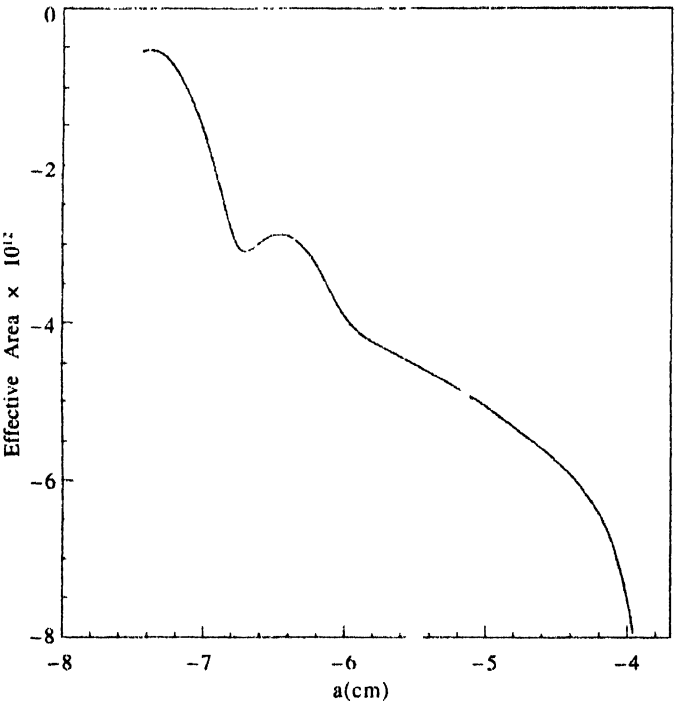

Figure 1. Variation of the effective surface area of the grains as a function of the radius of the grains.

~1–10 Angstrom, other with ~50–100 Angstrom and the third type is ~0.1–1 micron. In Figure 1, we show the effective surface area as a function of the radius of the grain. To obtain the effective surface area, we use the distribution of Weingartner and Draine [11] and multiplied by the surface area of these grains. We find that the smaller grains have larger effective area, since their number density is very high. We use the three main types of grains to carry out the computation relating to grain chemistry.

For the time being, we use the Master equation approach for the smallest grains as suggested by Biham *et al* [12] and Green *et al* [13] and the rate equation approach [14] for the larger two types of grains. This gives us the mass fraction of H_2 molecules formed due to grain surfaces as a function of the radius of grains.

4. Chemical evolution of the interstellar cloud

At $t = 0$, the chemical content of a cloud is dominated by hydrogen and very little amount of other constituents. The initial abundance of various species (in mass fraction) of a molecular cloud is chosen to be same as the abundance near solar neighbourhood [15], H : He : C : N : O : Na : Mg : Si : P : S : Cl : Fe = 0.64 : 0.35897 : 5.6 (–4) : 1.9(–4) : 1.81(–3) : 2.96(–8) : 4.63(–8) : 5.4(–8) : 5.79(8) : 4.12(–7) : 9.0(–8) : 1.08(–8), where, 10^a is written as 1.0(a). The rates of the chemical reactions are taken from UMIST database [9].

We now present a few pathways to complex molecules. The production of organic molecules in dense interstellar clouds can occur *via* gas phase. Exothermic ion molecular reactions are most probable (endothermic reactions are not possible in the cold conditions like interstellar medium). The initiating process is the cosmic ray induced ionization of H_2 [10] to yield mainly H_2^+, H_2^+ + Cosmic Ray H_2 + e– + Cosmic Ray.

This H_2^+ ion reacts with H_2 and produces H_3^+, which then reacts with carbon to produce the simplest hydrocarbon, $C + H_3^+ \rightarrow CH^+ + H_2$; $CH^+ + H_2 \rightarrow CH_2^+ + H$; $CH_2^+ + H_2 \rightarrow CH_3^+ + H$; $CH_3^+ + H_2 \rightarrow CH_5^+ + h\nu$; $CH_5^+ + e^- \rightarrow CH_4 + H$; again, this could similarly produce C_3H_3, C_2H_5, $C_6H_4^+$, C_2H_5, C_3H_7, C_3H_7O, C_2H_5O *etc.* which then can produce, $N + C_3H_3^+ \rightarrow HC_3NH^+ + H$.

Similarly, ammonia NH_3 can be produced, which then reacts, $CH_3^+ + NH_3 \rightarrow CH_3NH_3^+ + h\nu$; $CH_3^+ + HCN \rightarrow CH_3CNH^+ + h\nu$, which then produce methyl amine and aceto-nitrile *via* dissociative recombination reactions. The oxygen-containing organic molecules such as alcohol, acetaldehyde, dimethyl ether *etc.* can also be produced from the following reactions, $CH_3^+ + H_2O \rightarrow CH_3OH_2^+ + h\nu$; $H_3O^+ + C_2H_2 \rightarrow CH_3CHOH^+ + h\nu$; $CH_3^+ + CH_3OH$. $(CH3)_2OH^+ + h\nu$.

5. Results and comparison with observation

We present results of a typical model calculation. We start with a cloud of radius 1pc and let it collapse with velocity

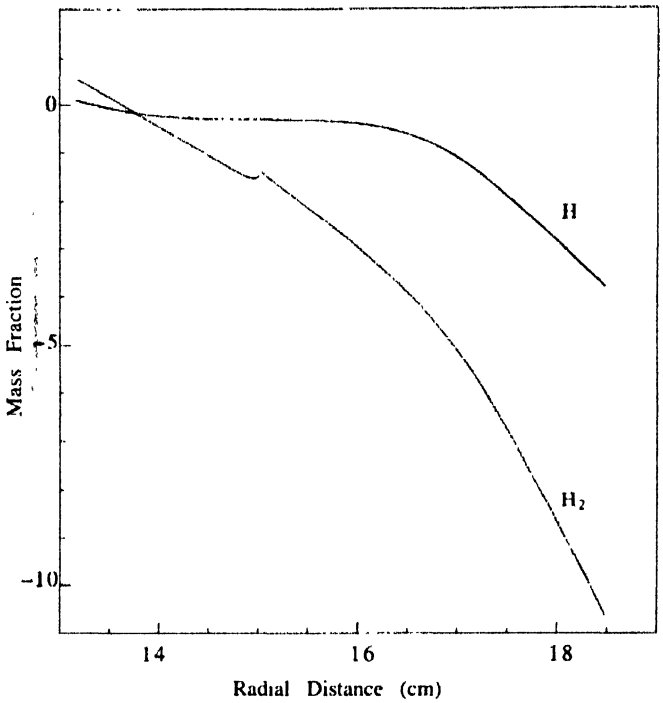

Figure 2. Variation of the saturation value of the expectation value of H and H_2 on the grain surface. The kink at ~10^{15} cm is an artefact at the junction of the adiabatic and isothermal phases of the gas.

and density as described in Section 2 above. Initial density is $\rho = 10^{-22}$ gm cm^{-3} and the temperature is 10°K. The angular velocity is $\Omega = 10^{-16}$ rad s^{-1}. At each stage of the collapse, chemical evolution is studied, first by following the grain-chemistry and then by gas chemistry. In Figure 2, we present the variation of the expectation value of H and H_2 on grain surface after saturation is achieved through processes such as adsorption and desorption. These numbers, when multiplied by the number density of grains (typically, 10^{-5}–10^{-12} of the number density of H in gas phase) gives the number density of H and H_2 in grain phase. In this analysis the grain temperature has been assumed to remain the same (10°K). In Figure 3, we present the mass fraction of H, H_2, and some other simple chemical species relevant to bio-molecule formation as a function of the radius of the collapsing cloud in a typical case. Except H, which is being used up in forming molecules, all the other species show tendency to have larger mass fraction as the collapse proceeds.

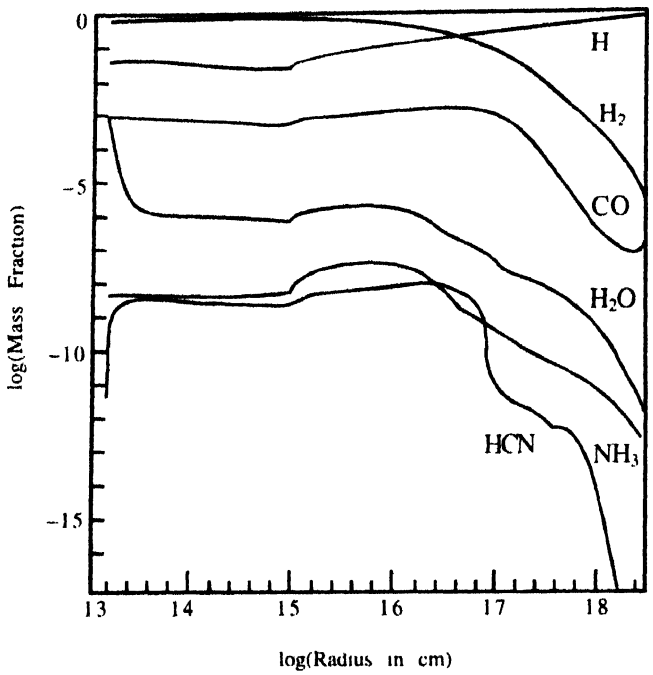

Figure 3. Variation of the mass fraction of a few simple molecules responsible for life formationas the could collapses from 1pc to 1AU.

Table 1. A comparison of the ratio of species from our model with that from observation of TMC.

Species ratio	Observed[1]	Computed[2,3]
$N(CO)/N(H_2)$	8×10^{-5}	1.4×10^{-4}
$N(HCN)/N(H_2)$	2×10^{-8}	8×10^{-9}
$N(NH3)/N(H_2)$	2×10^{-9}	2×10^{-9}

[1]Observation of TMC [16,17].

[2]Averaging over $r \sim 10^{15-16}$ cm for the case in Figure 3.

[3]Number densities are obtained from $N(X)=N_A\rho[X]/A_X$, where, $[X]$ is the mass fraction of the X-th species, N_A is the Avagadro's number and A_X is the atomic number of X-th species.

A number of workers have presented observations of molecular clouds, but the results vary from cloud to cloud. While the absolute abundance is not available, most of the observations refer to column densities of different species [17]. We present here a Table to indicate our number density ratios from Figure 3 and the observed abundance ratios. We assume the abundance to be an average value in the region around 10^{15} to 10^{16} cm.

Our computed value is consistent with the observations of TMC cloud, although variation from cloud to cloud may be up to 2–3 orders of magnitude, in general. Given this similarity, we believe that our computation of the light species is generally correct and we could now proceed in computing more complex bio-molecules.

6. Concluding remarks

In the paper, we have shown that simple bio-molecules can be produced during collapsing interstellar cloud. We have taken great care in computing the formation of H_2 molecules through grain chemistry, by properly choosing the size of the grains and then using master equation for grains of small size and rate equation for grains of large size. In reality, when the expectation value is large, one could use rate equations for all the grains. This is a major improvement over and above the earlier work of Chakrabarti and Chakrabarti [2]. In that work, the grain chemistry of H + H $\rightarrow$ H_2 was taken care of by using an effective rate constant [15] without explicitly doing the grain chemistry.

We have also compared our results with the observed ratios of number densities of various species and found them to be consistent. Our code appropriately followed chemical reaction at every radial distance during core collapse. In future, this would be used to check if complex bio-molecules could also be produced. The work is supported in part by a grant from Indian Space Research Organization (ISRO).

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